Resolution Function
of
SANS Diffractometer
with
Refractive Lenses

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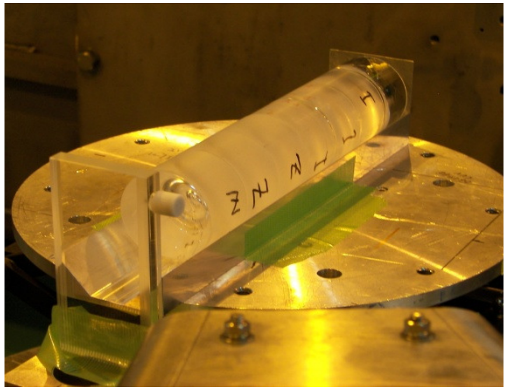
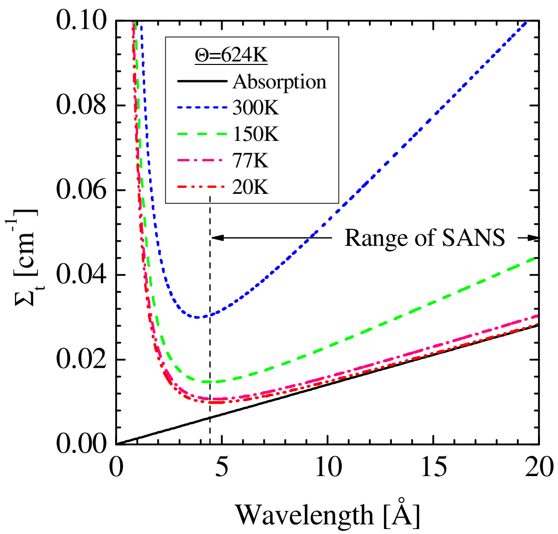
Components: Neutron Lenses



Purchased from Zeiss
and Ingeneric (Aachen)

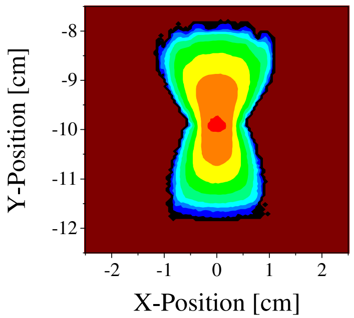
full sets KWS1/2 (2x26)



Effects of phonon scattering calculated

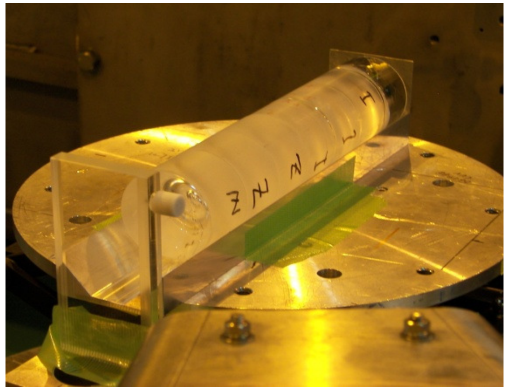
Lenses will be cooled to ~70K

Cooled lens holder in construction.

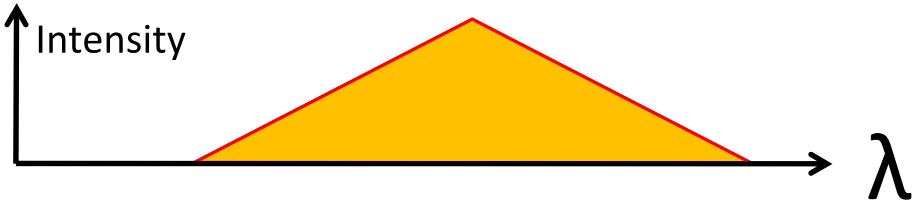


Simulation routines for
McStas and Vitess existing.

Resolution of Neutron Lenses



Wavelength Distribution from Selector

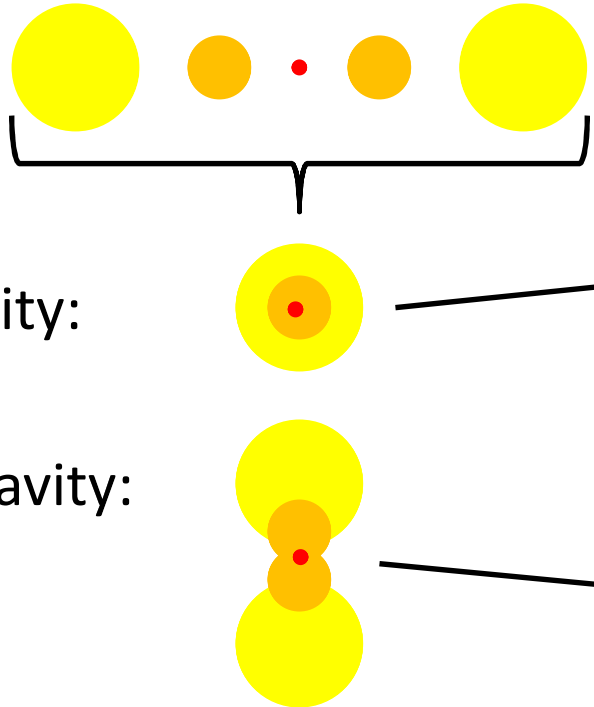


Simulations:

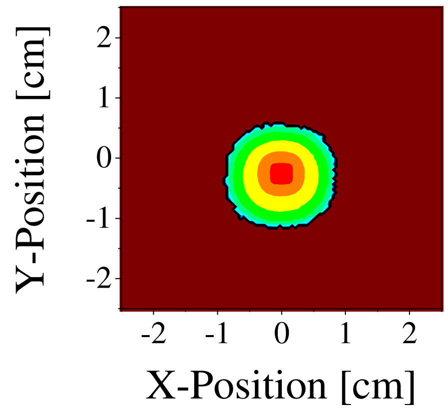
Focus:

No Gravity:

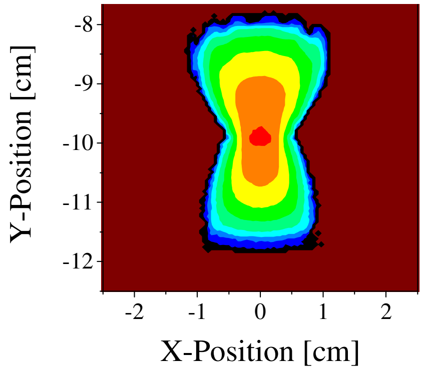
With Gravity:
(peanut)



little gravity

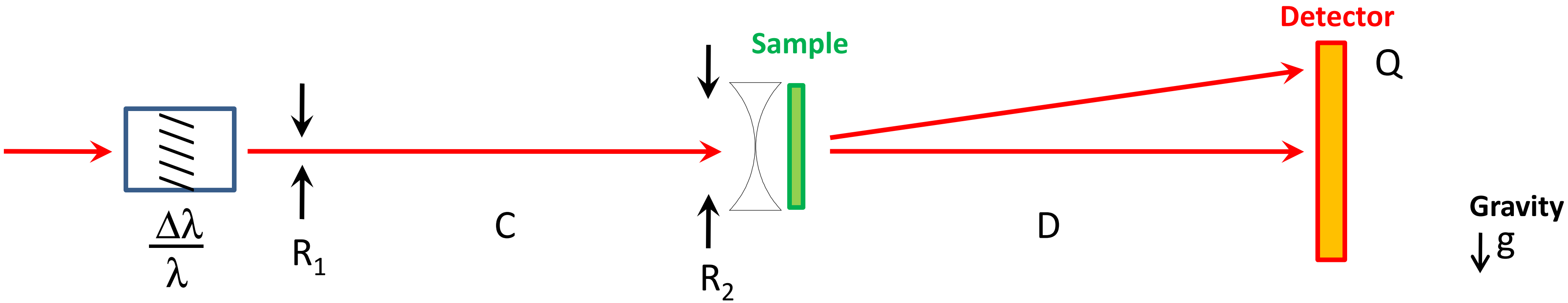


strong gravity



Strength of this effect $\sim \lambda^2 D^2$ i.e. strongest for low Q.

1st step of resolution correction: isotropic, rad. averaged



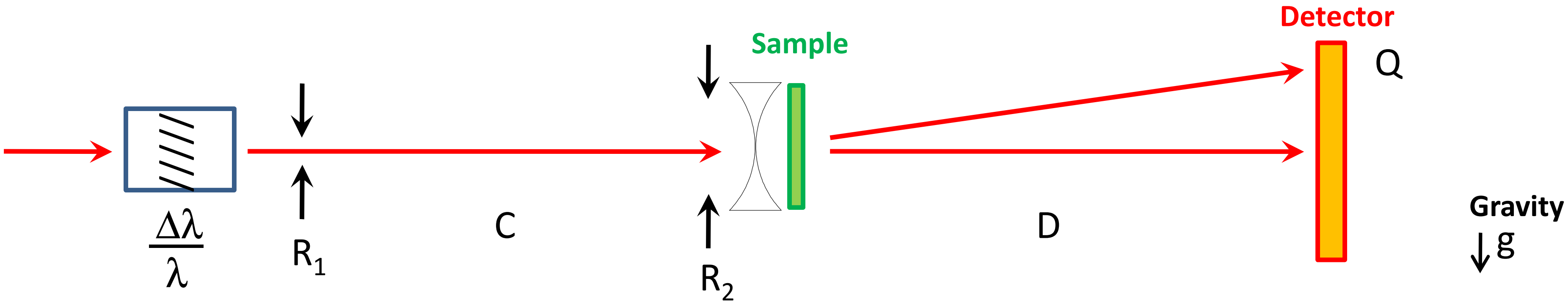
$$\sigma_Q^2 = a_1 \cdot R_1^2 + \left(\frac{\Delta\lambda}{\lambda}\right)^2 \left(a_2 \cdot R_2^2 + a_3 \cdot g^2 + a_4 \cdot Q^2\right) + \text{crossterms}(^4)$$

small negligible for classical SANS

to Pedersen Resolution Function

a_1, a_2, a_3, a_4 (C,D, …) determined by analytical calculations *and* computer simulations (McStas) done

1^{st} step of resolution correction: isotropic, rad. averaged



Abbrevations:

$$r_1 = \frac{2\pi}{\lambda D} \cdot \frac{D}{C} \cdot R_1$$

5E-4 .. 5E-5

$$r_2 = \frac{2\pi}{\lambda D} \cdot 2 \cdot \left(1 + \frac{D}{C}\right) \cdot R_2$$

9E-3

actually diameters !

$$q_0 = \frac{2\pi}{\lambda D} \cdot D \cdot (C + D) \cdot \frac{g m_n^2}{2h^2} \cdot \lambda^2$$

5E-4

$$Q$$

1E-3 .. 1E-4

Simulations with McStas

Radial averaging of a Debye-Scherrer ring

$\Delta Q(r_1)$ from (r_1 varied, r_2 small, gravity off, fixed angle)

$\Delta Q(r_2)$ from (r_1 small, r_2 varied, gravity off, fixed angle)

$\Delta Q(g)$ from (r_1 small, r_2 small, gravity varied, fixed angle)

$\Delta Q(Q)$ from (r_1 small, r_2 small, gravity off, real scattering)

Summary of resolution functions:

$$\sigma_Q^2 = 0.125 \cdot r_1^2 + \left(\frac{\Delta\lambda}{\lambda}\right)^2 \left(0.021 \cdot r_2^2 + 0.667 \cdot q_0^2 + 0.333 \cdot Q^2\right)$$

Mildner

$$\sigma_Q^2 = 0.250 \cdot r_1^2 + \left(\frac{\Delta\lambda}{\lambda}\right)^2 \left(0.016 \cdot r_2^2 + 0.472 \cdot q_0^2 + 0.236 \cdot Q^2\right)$$

Analytical O(Q^2)

$$\sigma_Q^2 = 0.250 \cdot r_1^2 + \left(\frac{\Delta\lambda}{\lambda}\right)^2 \left(0.008 \cdot r_2^2 + 0.173 \cdot q_0^2 + 0.086 \cdot Q^2\right)$$

Analytical O(Q^4)

$$\sigma_Q^2 = 0.107 \cdot r_1^2 + \left(\frac{\Delta\lambda}{\lambda}\right)^2 \left(0.026 \cdot r_2^2 + 0.096 \cdot q_0^2 + 0.242 \cdot Q^2\right)$$

Simulations McStas

$\Delta Q(r_1)$ = 1.6E-4	$\Delta Q(r_2)$ = 1.5E-4	$\Delta Q(g)$ = 1.5E-5	$\Delta Q(Q)$ = 0.5E-4	Classical SANS
$\Delta Q(r_1)$ = 1.6E-5	$\Delta Q(r_2)$ = 1.5E-4	$\Delta Q(g)$ = 1.5E-5	$\Delta Q(Q)$ = 0.5E-5	focussing SANS

2nd step of resolution correction: higher order terms

$$f\begin{pmatrix}\delta q_x\\ \delta q_y\end{pmatrix} = \exp\left[-\begin{pmatrix}\sigma_x^{-2}\\ \sigma_y^{-2}\end{pmatrix}\begin{pmatrix}\delta q_x^2\\ \delta q_y^2\end{pmatrix}\right]\cdot\left(1+\begin{pmatrix}A_x\\ A_y\end{pmatrix}\begin{pmatrix}\delta q_x^2\\ \delta q_y^2\end{pmatrix}+\begin{pmatrix}\delta q_x^2\\ \delta q_y^2\end{pmatrix}\begin{pmatrix}B_{xx} & B_{xy}\\ B_{yx} & B_{yy}\end{pmatrix}\begin{pmatrix}\delta q_x^2\\ \delta q_y^2\end{pmatrix}\right)$$

1st order resolution function (as before) — slight corrections — **Peanut** corrections

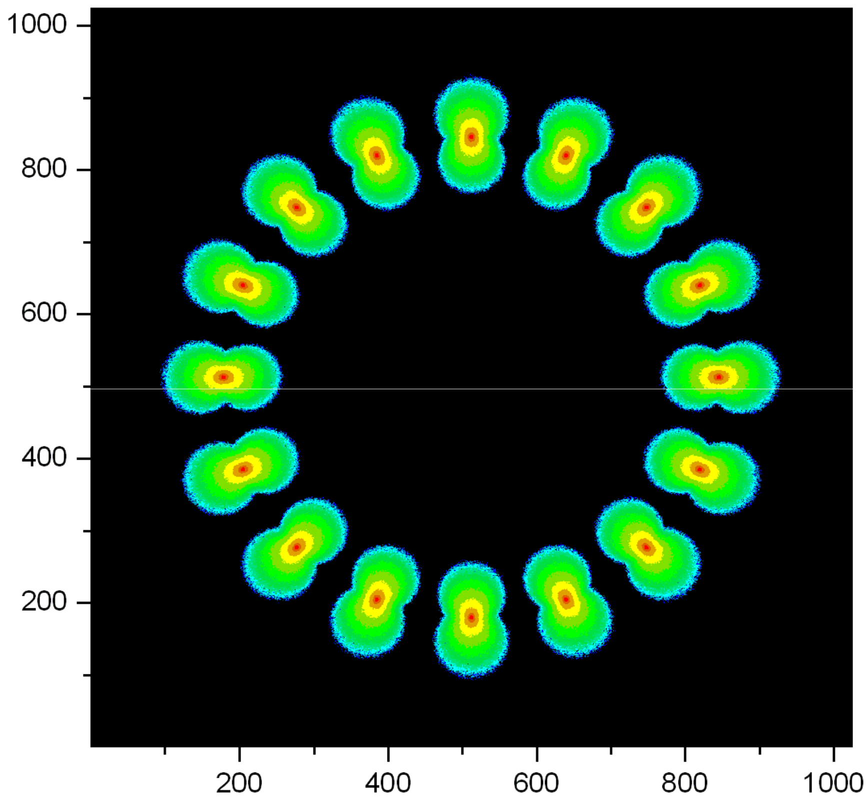
a) Fit of smeared theoretical function

b) Desmearing of measured spectrum

Current status:

Most important dependence of A,B (R_1,R_2,g,Q) needs to be determined (analytically & from simulation)

No Gravity



With Gravity